1-Propene, 3,3-dichloro-2-chloromethyl

Inchi: InChI=1S/C4H5Cl3/c1-3(2-5)4(6)7/h4H,1-2H2
InchiKey: BKSGSFFPKXGKBD-UHFFFAOYSA-N
Formula: C4H5Cl3
SMILES: C=C(CCl)C(Cl)Cl
Mol. weight [g/mol]: 159.44

Physical Properties

Property code	Value	Unit	Source
gf	23.86	kJ/mol	Joback Method
hf	-62.75	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	36.67	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.585		Crippen Method
mcvol	99.640	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinpol	918.00		NIST Webbook
rinpol	918.00		NIST Webbook
tb	399.33	K	Joback Method
tc	602.68	K	Joback Method
tf	193.88	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.34	J/mol×K	399.33	Joback Method
cpg	156.00	J/mol×K	433.22	Joback Method
cpg	162.27	J/mol×K	467.11	Joback Method
cpg	168.14	J/mol×K	501.00	Joback Method
cpg	173.65	J/mol×K	534.90	Joback Method
cpg	178.81	J/mol×K	568.79	Joback Method
cpg	183.64	J/mol×K	602.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R12408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume